Chemical Equilibrium Code

Equation-of-state code for calculating multiphase equilibrium properties

As a national resource for energetic materials, LLNL has long had an ongoing need to understand and predict the behavior of high explosives. To meet this need, the Laboratory developed—and continues to refine—the CHEQ (CHemical EQuilibrium) equation-of-state code.

A versatile calculation tool

CHEQ can calculate the equilibrium thermodynamic quantities of multiphase mixtures. It also calculates a variety of different states:
- Standard states: (T,P), (T,ρ), (S,P), (S,ρ), (E,P), (H,P), (G,P), and (Hugoniot,P)
- Nonstandard states: (T,S) and (ρ,P)
- Special states: CJ and non-CJ detonations.

Operating features

CHEQ uses modern statistical mechanical models to calculate thermodynamic quantities. It calculates the equation of state of fluids at a given temperature and pressure using an effective one-component fluid model. The code uses a statistical mechanical-variation perturbation theory to optimize the hard-core diameter of a hard-sphere reference fluid. CHEQ also incorporates several different solid-state models. Especially useful in the study of explosives is its three-phase (diamond, graphite, and liquid) model for carbon. CHEQ adjusts the composition in the multiple fluid and solid phases until it achieves minimum Gibb's free energy. This defines all thermodynamic properties at a given (T,P) point in phase space. For more complicated calculations (such as constant entropy, Hugoniot, Chapman–Jouget, and pressure–volume states), CHEQ calculates a number of (T,P) points until the desired state is determined.
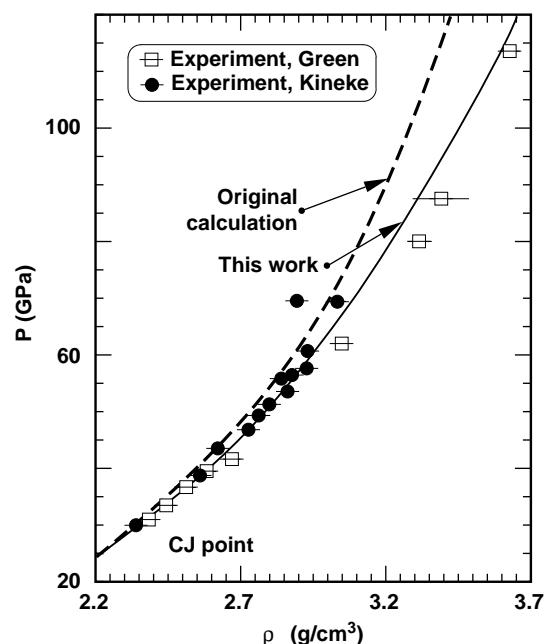
The advanced theoretical nature of CHEQ allows it to accurately model experimental data. This figure compares an earlier theoretical interpretation and the improved modeling interpretation with CHEQ of experimental data for PETN, a high explosive.

APPLICATIONS

- Prediction of pressure–volume relations of explosives and combustion products
- Determination of detonation properties of explosives

Simple graphic interface available

MXCHEQ, an X11-Motif-based controller, is also available with CHEQ on a variety of platforms to provide the user with a simple graphic interface to CHEQ. MXCHEQ can create the input file, run the program, and access the data files when the job is finished.

Availability: CHEQ is available now; LLNL is seeking industrial partners for moving the application of this technology into industry.

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